Funding boosts exascale computing research

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Los Alamos projects help set path to next-generation supercomputers

LOS ALAMOS, N.M., Sept. 7, 2016—In today's Department of Energy Exascale Computing Project (ECP) funding announcement, six Los Alamos National Laboratory partnership projects were tagged for full funding and one for seed money. The projects, all collaborations with other national laboratories and universities, target advanced modeling and simulation solutions to specific challenges supporting key DOE missions in science, clean energy and national security, as well as collaborations such as the National Cancer Institute's Precision Medicine Initiative.

"Our collaborative role in these exascale applications projects stems from our laboratory's long-term strategy in co-design and our appreciation of the vital role of high-performance computing to address national security challenges," said John Sarrao, associate director for Theory, Simulation and Computation at Los Alamos National Laboratory.

"The opportunity to take on these scientific explorations will be especially rewarding because of the strategic partnerships with our sister laboratories," Sarrao said.

Codesign is developing the interacting components of a computational system as a whole. The overall awards will be funded in the following strategic areas: energy security, economic security, scientific discovery, climate and environmental science, and healthcare.

"These application-development awards are a major first step toward achieving mission-critical application readiness on the path to exascale," said ECP director Paul Messina.

Exascale refers to high-performance computing systems capable of at least a billion billion calculations per second, or a factor of 50 to 100 times faster than the nation's most powerful supercomputers in use today.

The application efforts will help guide DOE's development of a U.S. exascale ecosystem as part of President Obama's National Strategic Computing Initiative (NSCI). DOE, the Department of Defense and the National Science Foundation have been designated as NSCI lead agencies, and ECP is the primary DOE contribution to the initiative.

The ECP's multi-year mission is to maximize the benefits of high-performance computing (HPC) for U.S. economic competitiveness, national security and scientific discovery. In addition to applications, the DOE project addresses hardware, software, platforms and workforce development needs critical to the effective development and deployment of future exascale systems.

Leadership of the Exascale Computing Project comes from six DOE national laboratories: The Office of Science's Argonne, Lawrence Berkeley, and Oak Ridge national labs, and NNSA's Los Alamos, Lawrence Livermore, and Sandia national labs.

The list of application development awards for Los Alamos is as follows:

Full Funding:

- Molecular Dynamics at the Exascale: Spanning the Accuracy, Length and Time Scales for Critical Problems in Materials Science, Arthur Voter (LANL) with SNL, University of Tennessee
- Computing the Sky at Extreme Scales, Salman Habib (ANL) with LANL, LBNL
- Exascale Deep Learning and Simulation Enabled Precision Medicine for Cancer, Rick Stevens (ANL) with LANL, LLNL, ORNL, NIH/NCI
- Transforming Additive Manufacturing through Exascale Simulation (TrAMEx), John Turner (ORNL) with LLNL, LANL, NIST
- Data Analytics at the Exascale for Free Electron Lasers, Amedeo Perazzo (SLAC) with LANL, LBNL, Stanford
- Cloud-Resolving Climate Modeling of the Earth's Water Cycle, Mark Taylor (SNL) with ANL, LANL, LLNL, ORNL, PNNL, UCI, CSU

Seed Funding

- Exascale Solutions for Microbiome Analysis, Kathy Yelick (LBNL) with LANL, Joint Genome Institute

About ECP

The ECP is a collaborative effort of two DOE organizations—the Office of Science and the National Nuclear Security Administration. As part of President Obama's National Strategic Computing Initiative, ECP was established to develop a capable exascale ecosystem, encompassing applications, system software, hardware technologies and architectures, and workforce development to meet the scientific and national security mission needs of DOE in the mid-2020s timeframe.